ISOLATED 1,4-NAPHTHOQUINONE AND ITS STEP-WISE MICROSOLVATION IN THE GAS PHASE: STRUCTURE AND BINDING BY ROTATIONAL SPECTROSCOPY

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1,4-Naphthoquinone (NTQ) is an important product of naphthalene oxidation and it also appears as a motif in many biologically active compounds. NTQ is introduced into the atmosphere by direct emissions from combustion of organic matter, and as a result of reactions of polycyclic aromatic hydrocarbons in the troposphere. Here we present a study of NTQ and its interactions with water using broadband rotational spectroscopy. Bare NTQ and its complexes with one, two and three water molecules have been detected. Their structures and relative arrangements have been determined by using ^{18}O isotopic data aided by theoretical calculations. Water molecules have been found to adapt their arrangement with respect to NTQ to maximise primary and secondary interactions, with more efficient competition between in-plane and above-plane complex configurations as the number of water molecules increase.